Nonlinear rotating modes: Green's-function solution

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(Received 28 May 1996; revised manuscript received 17 October 1996)

Lattice Green's functions are used to investigate localized rotating modes recently exhibited in some nonlinear lattices. For a one-dimensional lattice, analytical expressions of the solution are obtained, first in the rotating-wave approximation and then by including higher-order terms. Numerical simulations confirm the validity of these solutions. The method is not restricted to one-dimensional lattices. [S1063-651X(97)03202-9]

PACS number(s): 03.20.+i, 03.40.Kf, 63.20.Ry

I. INTRODUCTION

The recent surge of interest in nonlinear energy localization in homogeneous discrete lattices [1–3] has attracted attention on local *oscillatory* modes, or discrete breathers. They appear even more ubiquitous than the solitons [4] because they do not have a threshold energy and thus bridge the gap between the linear phonon modes and the highly nonlinear modes. Moreover, in some systems, discrete breathers are easily thermally activated [5,6] so that they are likely to be physically relevant. MacKay and Aubry have recently proved that breathers are exact solutions of nonlinear lattices if the intersite coupling is below a threshold which depends on the amplitude of the mode [7].

But oscillatory modes are not the only nonlinear localized modes. In lattices of coupled rotators we recently exhibited *rotating modes* [8] in which a central rotator performs a monotone increasing rotation while its neighbors oscillate around their equilibrium positions. In the phase space of the system, the motion of the central site and the motion of the neighbors lie on opposite sides of a separatrix. As a result the rotating modes are intrinsically discrete. There is no smooth way to go from a full rotation to an oscillation. The theorem of MacKay and Aubry [7] can be extended to show that rotating modes can be exact solutions of the coupled-rotator equations of motions, and numerical investigations of the thermalization of the rotator lattice [8] show that, like the breathers, the rotating modes can be thermally excited. Moreover, while it is very easy to thermally excite rotating modes that involve one or a few lattice sites, nonlocalized rotating modes are not observed unless one reaches very high temperatures because they have a very large energy. This is a sharp contrast with oscillatory modes for which the nonlocalized counterparts, i.e., oscillatory waves, or phonons, are easily found. As a result, in physical systems, such as plastic crystals, where rotations have been found experimentally [9,10], it seems very likely that they correspond to localized rotating modes. This is why it is important to have a mathematical description of these modes.

However, due to the specificity of the rotating modes, getting an analytical solution turns out to be much more difficult than for oscillatory modes because there is a qualitative change between the motion of the central site and the oscillations of the others. This precludes any continuum limit, and different functions must be used to describe the dynamics of different sites. In a previous work [8], we showed how an approximate solution could be derived. Numerical checks have indicated that this solution was rather good because it treated intrinsically the discreteness of the lattice. However, the method that we used was strictly limited to a one-dimensional lattice. We present here a solution based on lattice Green's function. The numerical solution that can be deduced from the analytical expressions given by the Green's functions is slightly better than the previous one, but, more importantly, the method is not restricted to one-dimensional lattices and can be formally extended to two or three dimensions, although the calculations could become involved. Section II presents the model and the solution derived in the rotating-wave approximation. Section III goes beyond this approximation and discusses the results.

II. MODEL AND GREEN'S-FUNCTION SOLUTION IN THE ROTATING-WAVE APPROXIMATION

We consider the one-dimensional sine-lattice equation

$$J[\sin(u_{n+1}-u_n)-\sin(n_n-u_{n-1})]-\frac{d^2u_n}{dt^2}=g\sin u_n \quad , \qquad (1)$$

where u_n is the field variable associated to the nth site of the lattice, and J, g are constants. This set of equations describes the dynamics of a chain of coupled rotators (pendula or molecules in a plastic crystal) with Hamiltonian

$$H=\sum_n \left\{ \frac{I}{2}\left(\frac{du_n}{dt}\right)^2 + K[1-\cos(u_{n+1}-u_n)] + V[1-\cos u_n]\right\}, \qquad (2)$$

where I is the moment of inertia of a rotator, K and V the magnitude of the coupling and on-site potentials, with

$J=K/I$ and $g=V/I$. One should notice that, instead of the usual harmonic coupling between sites, we consider here a sinusoidal coupling which is relevant, for instance, for dipolar interactions. This is a crucial property of the model because it allows for the existence of localized rotating modes. The monotonous rotation of a single site, while the neighbors oscillate, does not cause a permanent buildup of coupling energy. Moreover, as the coupling potential is bounded, the rotating modes are highly localized for all J/g. This determines the approach that can be used to look for a solution.

Let us rewrite Eq. (1) under the form

$$\frac{d^2u_n}{dt^2}=-[g+J(\cos u_{n+1}+\cos u_{n-1})]\sin u_n + J\cos u_n[\sin u_{n+1}+\sin u_{n-1}] \quad . \tag{3}$$

Equation (3) can be viewed as a modified version of the equation of motion of the nth pendulum with an effective frequency

$$\omega_0^*=[g+J(\cos u_{n+1}+\cos u_{n-1})]^{1/2} \quad , \tag{4}$$

coupled to its neighbors by an effective coupling constant

$$J^*=J\cos u_n \quad . \tag{5}$$

Let us look for a particular solution in which a single rotator (say, $n=0$) undergoes a rotational motion while the others oscillate. This means that

$$|u_0|\gg|u_n| \quad \text{for} \quad |n|\geqslant 1 \quad . \tag{6}$$

As we expect a highly localized solution, we preserve the full nonlinearity of the equations for the central site only while the other equations are linearized around the equilibrium position, which yields

$$\frac{d^2u_0}{dt^2}=-\omega_0^2\sin u_0+J(u_1+u_{-1})\cos u_0 \quad , \tag{7a}$$

$$\frac{d^2u_{\pm 1}}{dt^2}=-[g+J(1+\cos u_0)]u_{\pm 1}+J[u_{\pm 2}+\sin u_0] \quad , \tag{7b}$$

$$\frac{d^2u_n}{dt^2}=-\omega_0^2u_n+J(u_{n+1}+u_{n-1}), \quad |n|\geqslant 2 \, , \tag{7c}$$

where $\omega_0=\sqrt{g+2J}$ is the eigenfrequency of a single pendulum in the small amplitude limit.

Let us look for a solution of this set of equations under the form

$$u_0=v_{0,0}\,t+\sum_{r=1}^{\infty} v_{0,r}\sin(r\omega t) \quad , \tag{8a}$$

$$u_n=\sum_{r=1}^{\infty} v_{n,r}\sin(r\omega t) \quad \text{for} \quad |n|\geqslant 1 \quad . \tag{8b}$$

This expression is chosen to match the type of motion that we are looking for. The central rotator is expected to behave almost like a free rotating pendulum, i.e., rotate with an average velocity $v_{0,0}$, modulated by the on-site potential which tends to favor the positions $u_0=0 \pmod{2\pi}$, while the other sites will be driven to oscillate around equilibrium at a frequency imposed by the central rotator. It is also convenient to express $\sin u_0$ and $\cos u_0$ as

$$\sin u_0=\sum_{r=1}^{\infty} S_{0,r}\sin(r\omega t) \quad , \tag{9a}$$

$$\cos u_0=C_0+\sum_{r=1}^{\infty} C'_{0,r}\cos(r\omega t) \quad . \tag{9b}$$

The coefficients $v_{n,r}$, C_0, $C'_{0,r}$, $S_{0,r}$ ($n=0,\pm 1,\pm 2,\ldots,\pm\infty$, $r=1,\ldots,\infty$) and ω are parameters to be determined. Inserting Eqs. (8) and (9) into the equations of motions (7) we get a set of equations that couple these parameters. In a first step we confine ourselves to the ''rotating-wave approximation,'' often used to derive breather modes, which amounts to retaining only the leading terms, i.e., the terms up to $r=1$. We obtain

$$\omega^2 v_{0,1}=\omega_0^2 S_{0,1}-JC_0(v_{1,1}+v_{-1,1}) \quad , \tag{10a}$$

$$\omega^2 v_{\pm 1,1}=v_{\pm 1,1}[g+J(1+C_0)]-J(S_{0,1}+v_{\pm 2,1}) \quad , \tag{10b}$$

$$\omega^2 v_{n,1}=\omega_0^2 v_{n,1}-J(v_{n+1,1}+v_{n-1,1}) \quad , \quad |n|\geqslant 2 \quad . \tag{10c}$$

In the remainder of this section we drop the second subscript 1 ($v_{n,1}, S_{0,1}$ will be denoted as v_n, S_0, respectively) to simplify the notation since only $r=1$ is considered in the rotating-wave approximation.

The set of equations (10) for v_n is equivalent to the equations that one would derive for a linear homogeneous lattice [described by Eq. (10c) for all n], subjected to external forces represented by v_0, C_0, S_0. If the forcing terms are known, the v_n can be calculated with the lattice Green's functions $G(n,\omega)$ solutions of

$$(\omega^2-\omega_0^2)G(n,\omega)+J[G(n+1,\omega)+G(n-1,\omega)]=\delta(n) \quad . \tag{11}$$

The Green's functions have been calculated for many lattices [11,12]. Consequently the calculations presented here for a one-dimensional lattice can be formally extended to higher dimensions although they could become tedious. For a N-particle one-dimensional lattice with periodic boundary conditions, $G(n,\omega)$ is given by

$$G(n,\omega)=\frac{1}{N}\sum_q \frac{e^{inq}}{\omega^2-\omega_0^2+2J\cos q} = \frac{2}{N}\sum_{q\geqslant 0}\frac{\cos nq}{\omega^2-\omega_0^2+2J\cos q} \quad , \tag{12}$$

where the wave vector q belongs to the first Brillouin zone ($q=2k\pi/N$, $-N/2<k\leqslant N/2$). In the limit of large N, the discrete sum over q can be replaced by an integral

$$G(n,\omega)=\frac{1}{\pi(\omega^2-\omega_0^2)}\int_0^{\pi}\frac{\cos nq}{1+a\cos q}dq \, , \tag{13}$$

with $a=2J/(\omega^2-\omega_0^2)$.

A localized solution, i.e., a Green's function such that $|G|\to 0$ if $|n|\to\infty$ exists only if $a^2<1$. This defines the allowed frequencies ω, which must lie outside of the phonon band $\omega_0^2(q)=\omega_0^2-2J\cos q$, i.e., $\omega^2<\omega_m^2=\omega_0^2-2J$ or $\omega^2>\omega_M^2=\omega_0^2+2J$. We denote, by $G_-(n,\omega)$ and $G_+(n,\omega)$, the expressions of the Green's function in the low and high frequency range, respectively. Using the value [13] of the integral (13), they can be written as

$$G_\pm(n,\omega)=\pm\frac{(\mp 1)^{|n|}\exp(-z|n|)}{2J\sinh(z)} \quad \text{with} \quad z>0,$$

$$z=\cosh^{-1}\left(\pm\frac{\omega^2-\omega_0^2}{2J}\right) \quad . \tag{14}$$

Separating in Eqs. (10a) and (10b) the part corresponding to the perfect lattice described by Eq. (10c) from the extra contributions, and according to the properties of the Green's function for linear equations, one can express the response v_n to these extra contributions at sites $0,+1,-1$ as

$$\begin{aligned} v_n=&G_\pm(n,\omega)[\omega_0^2(S_0-v_0)-J(C_0-1)(v_1+v_{-1})] \\ &+G_\pm(n-1,\omega)[J(C_0-1)v_1-J(S_0-v_0)] \\ &+G_\pm(n+1,\omega)[J(C_0-1)v_{-1}-J(S_0-v_0)] \quad , \end{aligned} \tag{15}$$

where the appropriate Green's function $G_\pm$ has to be chosen according to the frequency ω. Taking into account the definition (11) of the Green's function, we obtain

$$\begin{aligned} v_n=&(S_0-v_0)[\omega^2 G_\pm(n,\omega)-\delta(n)] \\ &+(1-C_0)v_1[(\omega^2-g)G_\pm(n,\omega)-\delta(n)] \quad . \end{aligned} \tag{16}$$

For $n=1$, Eq. (16) determines v_1 as a function of the properties of the central rotator

$$v_1=\frac{(S_0-v_0)\omega^2 G_\pm(1,\omega)}{1-(1-C_0)(\omega^2-g)G_\pm(1,\omega)} \quad . \tag{17}$$

Inserting Eq. (17) into Eq. (16) for $n\neq 0$, we obtain an equation giving the spatial localization of the nonlinear rotating modes

$$v_n=\frac{\omega^2 G_\pm(n,\omega)(S_0-v_0)}{1-(1-C_0)(\omega^2-g)G_\pm(1,\omega)} \quad . \tag{18}$$

The same calculation for $n=0$ gives a relation between ω and the parameters S_0 and v_0 that characterize the central site according to Eqs. (8) and (9),

$$\frac{S_0}{v_0}=\frac{\omega^2[G_\pm(0,\omega)+AG_\pm(1,\omega)]}{\omega^2 G_\pm(0,\omega)-1+A\omega^2 G_\pm(1,\omega)} \tag{19}$$

with

$$A=\frac{(1-C_0)[(\omega^2-g)G_\pm(0,\omega)-1]}{1-(1-C_0)(\omega^2-g)G_\pm(1,\omega)} \quad . \tag{20}$$

Within the rotating-wave approximation, Eqs. (17)–(20) determine completely the dynamics of the lattice for any $n\neq 0$ as a function of the motion of the central site $n=0$. If they are combined with the Eq. (7a), they give a self-consistent set of equations which can be used to obtain the rotating mode solution. The analytical solution of this set of equations is, however, difficult to derive and it might be meaningless to look for an exact solution while we have made approximations, such as the partial linearization of the original equations and the rotating-wave approximation. At the same level of accuracy, one can drop the last term of Eq. (7a) which amounts to assuming that the large amplitude motion of the central site is not perturbed by the small vibrations of the neighboring sites. The central rotator is simply described by

$$\frac{d^2u_0}{dt^2}+\omega_0^2\sin u_0=0, \tag{21}$$

which has an exact solution in terms of elliptic functions [14]. For a given lattice, the nonlinear rotating mode is a one-parameter excitation. It is convenient to characterize it by the angular velocity Ω_0 of the central rotator at its equilibrium position $u_0=0$. The solution of the rotating pendulum is then

$$\sin\frac{u_0}{2}=\mathrm{sn}\left(\frac{\Omega_0}{2}t,\kappa\right) \quad \text{or} \quad u_0(t)=2\,\mathrm{am}\left[\frac{\Omega_0}{2}t,\kappa\right], \tag{22}$$

where the modulus κ of the Jacobi elliptic functions sn and am is equal to

$$\kappa=2\omega_0/\Omega_0<1. \tag{23}$$

From this expression of u_0, we can determine all the necessary parameters to get $u_n(t)$ for any $n\neq 0$. The Fourier series expansion of the amplitude elliptic function [15] gives the expansion (8a) of u_0,

$$u_0=\frac{\pi\Omega_0}{2K}t+4\sum_{r=1}^{\infty}\frac{q^r}{r(1+q^{2r})}\sin r\frac{\pi\Omega_0}{2K}t, \tag{24}$$

where $K(\kappa)$ is the elliptic integral of the first kind, K' is the associated elliptic integral $K'=K(\sqrt{1-\kappa^2})$, and $q=\exp(-\pi K'/K)$. Equation (24) gives $v_0=4q/(1+q^2)$. The expression of $\sin u_0$ is easily derived from Eq. (21) and expansion (24)

$$\sin u_0=\sum_{r=1}^{\infty}\left(\frac{2\pi}{\kappa K}\right)^2\frac{rq^r}{r(1+q^{2r})}\sin r\frac{\pi\Omega_0}{2K}t, \tag{25}$$

so that $S_0=(2\pi/\kappa K)^2 q/(1+q^2)$, $S_0/v_0=(\pi/\kappa K)^2$. Finally $\cos u_0$ is derived from the Fourier series of $\mathrm{sn}[(\Omega_0 t/2),\kappa]$. Its constant term C_0 is

$$\begin{aligned} C_0&=1-\left(\frac{2\pi}{\kappa K}\right)^2\sum_{m=0}^{\infty}\frac{q^{2m+1}}{(1-q^{2m+1})^2} \\ &=1-\left(\frac{\pi}{\kappa K}\right)^2\sum_{m=0}^{\infty}\frac{1}{\sinh^2[(2m+1)\pi K'/2K]}. \end{aligned} \tag{26}$$

Introducing S_0/v_0 and C_0 into Eqs. (19) and (20) defines a relation between the frequency ω of the rotating mode and Ω_0. One should notice that, although we have deduced S_0, v_0, C_0 from an analytical expression for $u_0(t)$, Eq. (22),

valid for a central rotator uncoupled to the rest of the lattice, we *do not* assume that the frequency of the rotating mode is simply the angular frequency of the isolated rotator as we did in our previous work [8]. The rotating mode is a one-parameter solution which can be characterized by the value of Ω_0. The value of ω, obtained by solving Eq. (19) for a given Ω_0 *takes into account the coupling to the other sites.* The shape of the rotating mode away from the central site is given by the values v_n which are completely determined by Eq. (18), once ω is known. From Eq. (18) and expression (14), we get

$$v_n = \pm \frac{\omega^2}{2J\sinh z} \frac{4q}{1+q^2}\left[\left(\frac{\pi}{\kappa K}\right)^2 - 1\right] \times \frac{1}{1-(1-C_0)(\omega^2-g)G_{\pm}(1,\omega)} (\mp 1)^{|n|} e^{-z|n|}. \quad (27)$$

To complete the determination of the solution defined by Eq. (8) in the rotating-wave approximation, one can obtain $v_{0,0}$ from the relation $\Omega_0 = v_{0,0} + \omega v_1$, deduced from the expression of the velocity of the central site at time $t=0$. Figure 1 shows the extrema of oscillation, v_n $(n \neq 0)$, of the rotators for the parameters $J=1$, $g=2$ and two values of the frequency of the rotating mode, $\omega = 1.264\,91$ which belongs to the low frequency range and $\omega = 3.033\,15$ in the high frequency range. The amplitude of the vibrations away from the central rotating site decays as ρ^n with

$$\rho = \mp e^{-z} = \frac{1}{2J}[g + 2J - \omega^2 \mp \sqrt{(g+2J-\omega^2)-4J^2}] \quad . \quad (28)$$

This decay rate is the same as the one obtained in the previous solution [8] because it is determined by the properties of the linearized lattice. Except when ω is in the immediate vicinity of the phonon band ($\omega \approx \omega_m$ in the low frequency range or $\omega \approx \omega_M$ in the high frequency range, which correspond to unstable solutions [8]) where ρ approaches 1, the rotating modes are highly localized excitations, as shown on Fig. 1. In the high frequency range, the sign of the v_n's alternates, which corresponds to the usual ''optical'' character of modes above the top of the phonon band.

The validity of the solution has been tested by numerical integration of Eqs. (1) with an initial condition obtained from Eqs. (22) and (27). The integration is performed with a fourth-order Runge-Kutta scheme and a time step chosen to preserve the total energy to an accuracy of 10^{-6} for the total time interval investigated. The results are plotted in Fig. 2. The energy density

$$e_n = \frac{1}{2}\left(\frac{du_n}{dt}\right)^2 + \frac{1}{2}J[2-\cos(u_{n+1}-u_n)-\cos(u_n-u_{n-1})] + g[1-\cos u_n] \quad (29)$$

shows a sharp peak around the center of the rotating mode. During one period of the mode there is an exchange between the kinetic energy (maximum when the central rotator is at the position $u_0 = 0$) and the potential energy, which is accompanied by a small oscillation of the width of the energy density peak. Simultaneously the amplitude of the peak oscillates to conserve the total energy, i.e., the area under the peak. While Fig. 2(a), for the energy density, seems to indicate an almost exact solution, the plot of the angular velocities of the rotators shows that the initial condition radiates small amplitude waves away from the center, i.e., the solution is not exact. This is not surprising since it has been obtained in the rotating-wave approximation which neglects all high frequency terms. The case that we have chosen for Fig. 2 is one example where the limitations of the Green's function solution show up clearly. Higher g/J ratio, which gives more localized solutions, shows that the solution is in fact rather good. However, Fig. 2 points out the interest of going beyond the rotating-wave approximation.

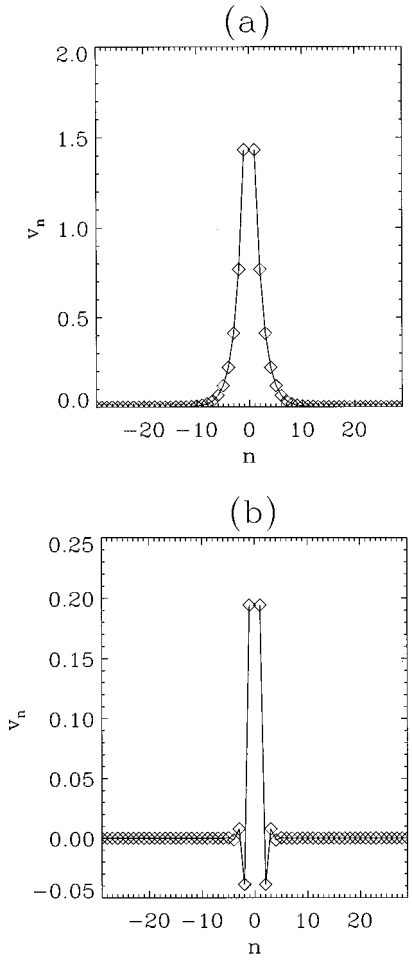

FIG. 1. Extrema of oscillation, v_n $(n \neq 0)$, of the off-center rotators for $J=1$, $g=2$, and $\omega = 1.264\,91$ (a) low frequency range and $\omega = 3.033\,15$ (b) high frequency range.

III. BEYOND THE ROTATING-WAVE APPROXIMATION

The next approximation is to keep terms up to the frequency 2ω in the analysis of Eqs. (7), and to identify the factors of $\sin\omega t$ and $\sin 2\omega t$. The $\sin\omega t$ terms give again the set of equations (10), and the $\sin 2\omega t$ terms give the additional equations

$$4\omega^2 v_{0,2} = \omega_0^2 S_{0,2} - J\frac{C'_{0,1}}{2}(v_{1,1}+v_{-1,1}) - JC_0(v_{1,2}+v_{-1,2}) \quad , \quad (30a)$$

$$4\omega^2 v_{\pm 1,2} = v_{\pm 1,2}[g + J(1+C_0)] - J(S_{0,2}+v_{\pm 2,2}) + J\frac{C'_{0,1}}{2}v_{\pm 1,1} \quad , \quad (30b)$$

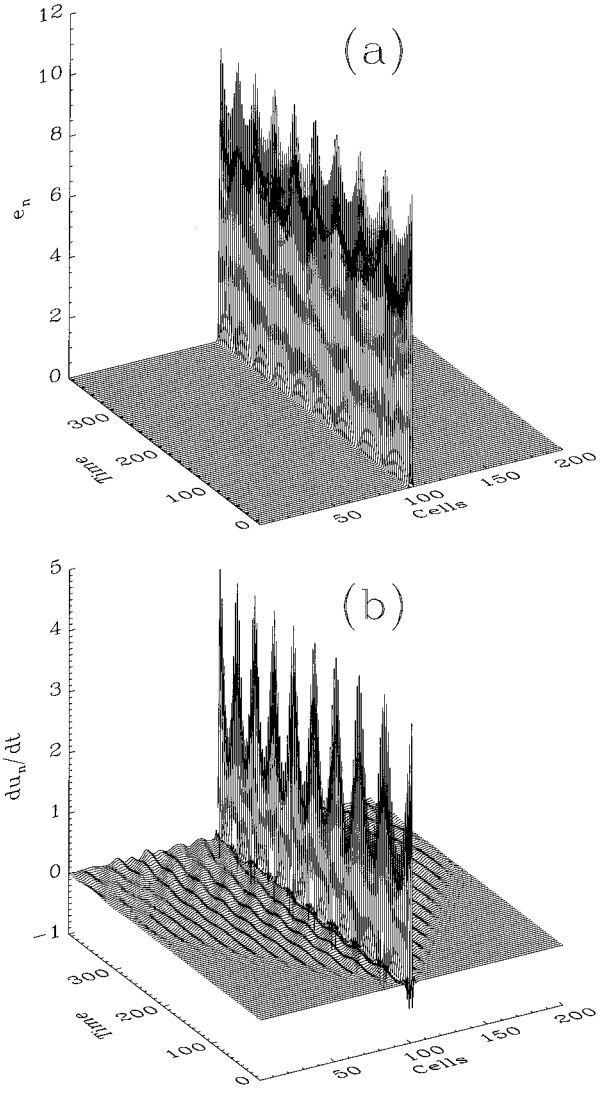

FIG. 2. Time evolution of an initial condition given by Eqs. (22) and (27) for $g=2$, $J=1$, $\omega=3.033\,15$. (a) Energy density e_n. (b) Angular velocities of the rotators. The amplitudes oscillate with the period of the rotating mode. The slow oscillation observed on the figure is an artifact due to a stroboscopic effect generated by the finite sampling time (much larger than the integration time step) which is necessary to generate a clear three-dimensional figure.

$$4\omega^2 v_{n,2}=\omega_0^2 v_{n,2}+J(v_{n+1,2}+v_{n-1,2}) \quad , \quad |n|\geqslant 2 \quad . \tag{30c}$$

This new set of equations couples the $v_{n,1}$ and $v_{n,2}$ terms. However, as the $v_{n,2}$ terms do not appear in Eqs. (10) which give the leading contribution to the solution, Eqs. (10) can be solved as before and $v_{n,1}$ is still given by the solution (27). Then, to calculate $v_{n,2}$ $(n\neq 0)$, the set of equations (30b) and (30c) can be treated as a set of linear equations forced by the external terms $S_{0,2}$ and $v_{\pm 1,1}$, which are known. It should be noticed that such a treatment of the equations is not fully self-consistent because it does not guarantee that Eq. (30a) will be exactly satisfied because ω is only determined by the lowest order set of equations (10). This is a limitation of the method which is inherent in our approach, which does not treat the central rotator and the remaining sites on an equal footing. It is justified by the fundamental difference between the large amplitude motion at the central site, which tends to drive the other rotators, and the small vibrations of the remaining sites. The validity of the approach is confirmed by the numerical tests of the solution.

Solving Eqs. (30) with the Green's function of the linearized lattice, which are the same as the functions calculated above simply taken for the frequency 2ω instead of ω, gives

$$\begin{aligned} v_{n,2}=G_{\pm}(n,2\omega)\Big[\omega_0^2(S_{0,2}-v_{0,2})-J(C_0-1)(v_{1,2}+v_{-1,2}) \\ -J\frac{C'_{0,1}}{2}(v_{1,1}+v_{-1,1})\Big]+G_{\pm}(n-1,2\omega)\Big[J\frac{C'_{0,1}}{2}v_{1,1} \\ +J(C_0-1)v_{1,2}-J(S_{0,2}-v_{0,2})\Big]+G_{\pm}(n+1,2\omega) \\ \times\Big[J\frac{C'_{0,1}}{2}v_{-1,1}+J(C_0-1)v_{-1,2}-J(S_{0,2}-v_{0,2})\Big] \quad . \end{aligned} \tag{31}$$

For the terms at frequency 2ω, Eq. (31) corresponds to Eq. (15) derived above for the terms at frequency ω. As the $v_{\pm 1,1}$ terms are known from the lowest order solution, Eq. (31) can be treated exactly as Eq. (15), except that ω is taken from the value determined above.

For the numerical tests of this solution including the 2ω corrections, we have, however, used a simplified version of Eq. (31) by dropping the $v_{\pm 1,1}$ contributions, i.e., assuming $C'_{0,1}=0$. This greatly simplifies the calculations and the neglected terms are, in fact, extremely small. It is easy to understand why when one looks at their physical origin. The $v_{n,2}$ terms are the response of the lattice to the 2ω term in the central rotator motion, which is not small, and to a 2ω contribution resulting from the nonlinear coupling between the central rotator and the vibration of the ± 1 sites. This second factor is small because, as shown above, the vibrations away from the center have a very small amplitude. Therefore, neglecting this higher order term is justified. Looking at Eq. (31) with $C'_{0,1}=0$, one can see that it is then exactly identical to Eq. (15). It means that $v_{n,2}$ is simply given by Eq. (18) and Green's function calculated for the frequency 2ω, i.e.,

$$v_{n,2}=\frac{4\omega^2 G_{\pm}(n,2\omega)(S_{0,2}-v_{0,2})}{1-(1-C_0)(4\omega^2-g)G_{\pm}(1,2\omega)} \quad , \tag{32}$$

which can easily be evaluated by replacing $S_{0,2}$ and $v_{0,2}$ by their values taken from expansions (25) and (24). In doing this evaluation, one should take care to use the appropriate Green's function $G_{\pm}$. The choice between G_- and G_+ is now determined by the value of 2ω. For high frequency rotating modes, ω being above the phonon band, this is also true for 2ω and the function G_+ can be used both for $v_{n,1}$ and $v_{n,2}$. But, for low frequency modes, it may happen that ω is below the phonon band, i.e., $v_{n,1}$ is calculated with G_-, but 2ω is above the phonon band and G_+ has to be used for $v_{n,2}$. Of course 2ω could fall *into* the phonon band. In this case $v_{n,2}$ would be determined by a *nonlocalized* Green's function. This means that the energy of the central

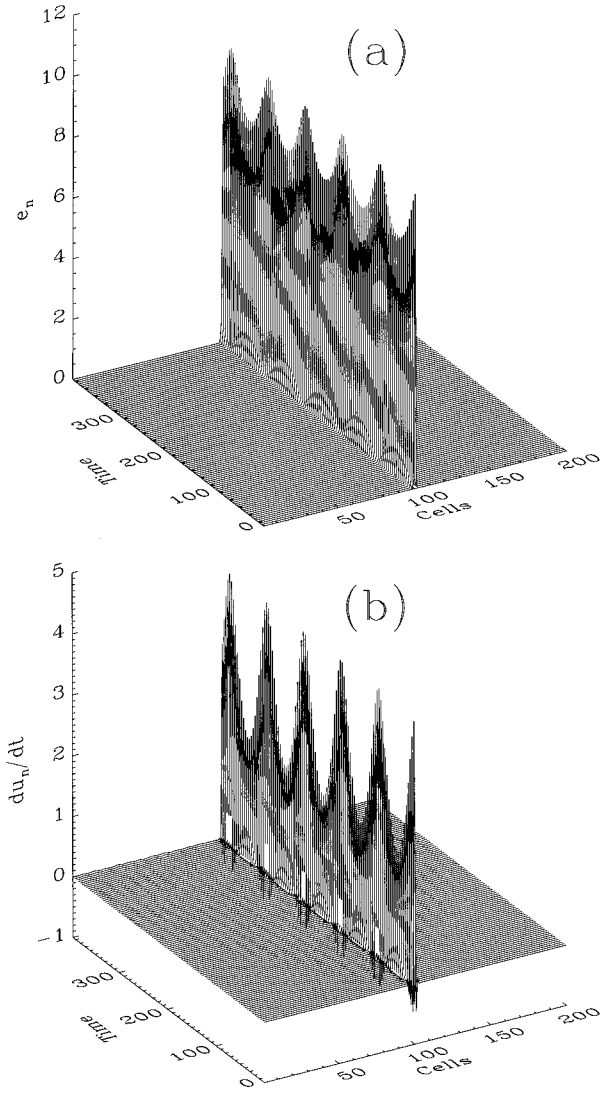

FIG. 3. Time evolution of an initial condition including the 2ω terms. The parameters are the same as in Fig. 2. The solution is almost exact. (a) Energy density e_n. (b) Angular velocities of the rotators.

rotator would constantly flow away from the center through linear waves at frequency 2ω and the rotating mode would be unstable. This provides an analytical justification for our previous numerical observations [8].

Figure 3 shows the time evolution of an initial condition including the $v_{n,1}$ and $v_{n,2}$ terms. The parameters are exactly the same as in Fig. 2. Note that the initial condition is now almost exact, showing the significant improvement brought by the introduction of the second harmonic 2ω in the solution.

The numerical simulations show therefore that a rather accurate expression of the rotating modes can be obtained with the lattice Green's function method. The starting point is to linearize the equations outside of the site that performs a continuous rotation. This approximation is justified by the *qualitative difference* between the motion of the center and that of the other sites, as well as by the small amplitude of the vibrations of the off-center sites, even in the case of a rather strong coupling such as the example $g/J=2$ chosen to illustrate the solution. This leaves only *one* nonlinear equation to solve, the equation that describes the rotation of the central site. In solving this equation, we again use the fundamental difference between the large amplitude motion of the center and the small vibrations of the other sites, which is consistent with the linearization already performed. This allows us to get an analytical expression for the rotation of the central site from the motion of an isolated rotator. However this does not amount to treating the central rotator as if it were really isolated because, although we use for $u_0(t)$ the functional expression of a single rotator, the calculation of the *frequency* of the rotation includes the coupling with the other sites. For a weak coupling case, the frequency correction can be small and this is why the numerical solutions obtained earlier with a method that ignored it were already rather good [8]. It is, however, important to have a method which can treat larger couplings, in particular, because some real physical systems where rotations have been investigated belong to this class [10]. The motion of the sites away from the center are calculated by a lattice Green's function method which can include successively the main frequency of the central rotation and its harmonics. We have shown that including the second harmonic brings a significant improvement. In principle, higher harmonics can be included in a similar way but it would become meaningless owing to the other approximations performed. Since the solution is obtained by linearizing the equations away from the center, it would be straightforward to generalize it to more complicated interactions, such as second-neighbor interactions that may be relevant for some real systems. This would simply require the introduction of the lattice Green's function appropriate for the new linearized equations. The only fundamental restriction on the interaction potential is that it must have a finite range and be a periodic function to allow one site to rotate while the neighbors oscillate without causing a monotonous increase of the coupling energy [8]. The main interest of the Green's function method is that it is not restricted to one-dimensional lattices. Lattice Green's functions have been obtained for a large variety of two- and three-dimensional lattices. Using these Green's functions, the one-dimensional calculations shown in this paper can be extended to higher dimensions. The only limitation is that multidimensional Green's function are generally not known analytically and consequently the rotating mode solution will only be known numerically. Work in this direction is in progress because the simulations of a thermalized lattice show that, when rotating modes are thermally created they are generally localized contrary to vibrational modes which show up first as phonons before local breathers can be formed. Moreover as molecular rotations have been detected experimentally in plastic crystals [9,10], it seems likely that nonlinear localized modes can exist in some real materials. It is therefore interesting to determine their properties.

ACKNOWLEDGMENTS

One of the authors (S.T.) would like to express his sincere thanks to Professor S. Homma and all other members in the Division of Physics, Faculty of Engineering, Gunma University, where part of this paper was done. M.P. would like to acknowledge the hospitality of the Gunma University, where this work was initiated. Work at Los Alamos is under the auspices of the U.S. D.O.E.

[1] A.J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[2] S. Takeno, K. Kisoda, and A.J. Sievers, Prog. Theor. Phys. Suppl. **94**, 242 (1988).
[3] J.B. Page Phys. Rev. B **41**, 7835 (1990).
[4] S. Takeno, J. Phys. Soc. Jpn. **61**, 2821 (1992).
[5] T. Dauxois, M. Peyrard, and A.R. Bishop, Phys. Rev. E **47**, 684 (1993).
[6] T. Dauxois and M. Peyrard, Phys. Rev. Lett. **70**, 3935 (1993).
[7] R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994); and S. Aubry (unpublished).
[8] S. Takeno and M. Peyrard, Physica D **92**, 140 (1996).
[9] L. Boyer, R. Vacher, L. Cecchi, M. Adam, and P. Bergé, Phys. Rev. Lett. **26**, 1435 (1971).
[10] F. Fillaux and C. J. Carlile, Phys. Rev. B **42**, 5990 (1990).
[11] S. Takeno, Prog. Theor. Phys. **28**, 33 (1962), and references therein.
[12] A.A. Maradudin, E.W. Montroll, and G.H. Weiss, in *Solid State Physics, Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic, New York, 1963), Suppl. 3.
[13] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1980).
[14] M. Toda, *Special Functions* (Asakura Shoten, Tokyo, 1981), Chap. 7 (in Japanese).
[15] P.F. Byrd and M.D. Friedman, *Handbook of Elliptic Integrals for Engineers and Physicists* (Springer-Verlag, Berlin, 1954).